Lattice QCD on Parallel Computers

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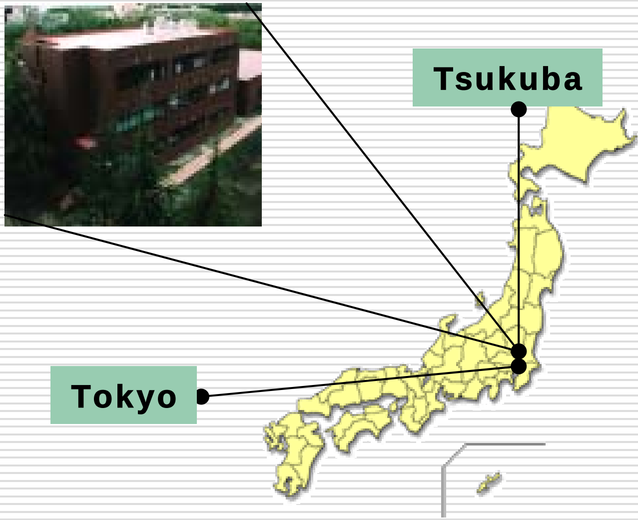
- *Lattice QCD and its goal*
- *Computers for lattice QCD*
- *Selected Physics achievements*
- *Future direction of lattice QCD and computational requirements*
- *Conclusions*

Center for computational Physics
University of Tsukuba

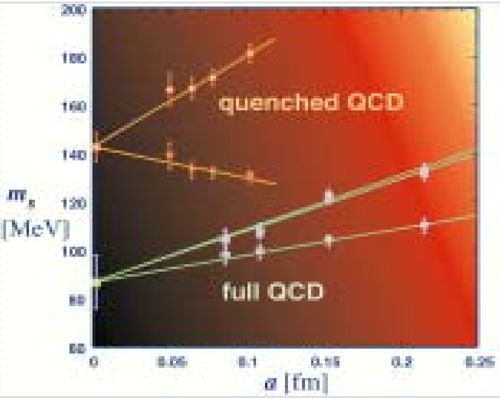
- Founded in 1992
- Emphasis on
  - Development of HPC systems suitable for computational physics
  - Close collaboration of physicists and computer scientists

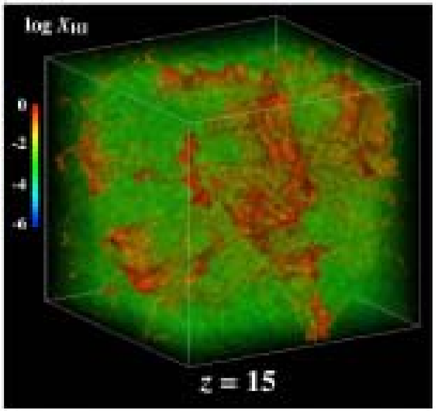


- Computing facility
  - CP-PACS parallel system
    - MPP with 2048PU/0.6Tflops peak
    - Developed at the Center with Hitachi Ltd.
    - #1 of Top500-November 1996
  - GRAPE-6 system
    - Dedicated to gravity calculations
    - Developed at U. Tokyo
    - 8Tflops equivalent

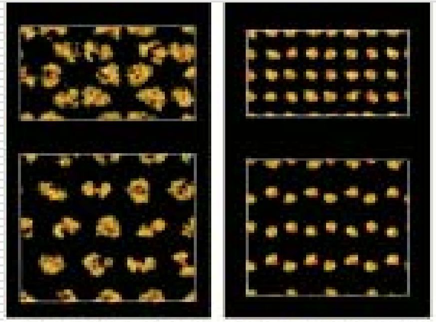
Computational physics at CCP

- Concentrated usage on a few fundamental physics problems which demands large-scale calculations





  - High energy physics; *Quantum Chromodynamics (QCD)*
  - Astrophysics; Radiation hydrodynamics
  - Condensed matter; phases of solid hydrogen



Phase I (T=300K, P=120GPa) Phase III (T=100K, P=180GPa)

Standard Model of elementary particles

- Particles:
  - 6 quarks $$\begin{pmatrix} u \\ d \end{pmatrix} \begin{pmatrix} s \\ c \end{pmatrix} \begin{pmatrix} t \\ b \end{pmatrix}$$
  - 6 leptons $$\begin{pmatrix} e \\ \nu_e \end{pmatrix} \begin{pmatrix} \mu \\ \nu_\mu \end{pmatrix} \begin{pmatrix} \tau \\ \nu_\tau \end{pmatrix}$$
- Interactions:
  - Strong interactions (nuclear force) — Quantum Chromo-Dynamics (QCD) SU(3)
  - Electromagnetic interactions
  - Weak interactions

} Glashow-Weinberg-Salam Theory SU(2)xU(1)

→ *Standard Model of quarks, leptons and their interactions*

Quantum Chromodynamics

- Fundamental theory of quarks and gluons and their strong interactions

$$S_{QCD} = \frac{1}{8\pi\alpha_s} Tr\left(F_{\mu\nu}F_{\mu\nu}\right) + \sum_f \overline{\psi}_f \left(\gamma_\mu \cdot \left(\partial_\mu - iA_\mu\right) + m_f\right)\psi_f$$

$$\left\langle O\left(A,\overline{\psi},\psi\right)\right\rangle = \frac{1}{Z}\int dA\,d\overline{\psi}\,d\psi\, O\left(A,\overline{\psi},\psi\right) e^{-S}$$

- Knowing

1 coupling constant α_s

and

6 quark masses $m_u, m_d, m_s, m_c, m_b, m_t$

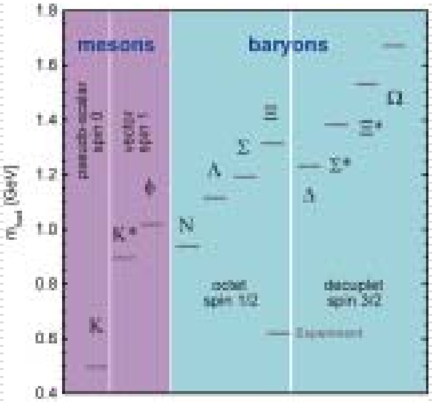
will allow full understanding of strong interactions

“Yukawa’s dream(1935) in modern form”

Physics goals of QCD

Understanding the hadron spectrum

Hadron physics



Determining the Fundamental constants of QCD

Natural Constants

- Strong coupling constant

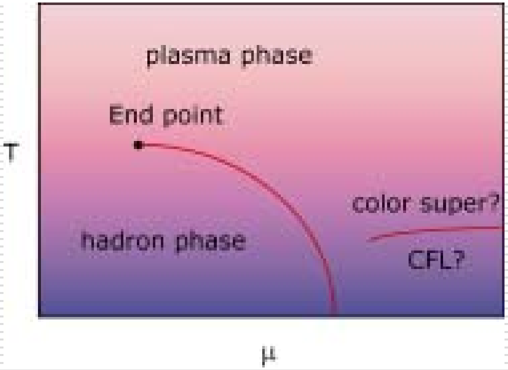
  α_s

- Quark masses

  $m_u, m_d, m_s, m_c, m_b, m_t$

Behavior of matter under extreme temperature and/or density

Physics of quark-gluon plasma

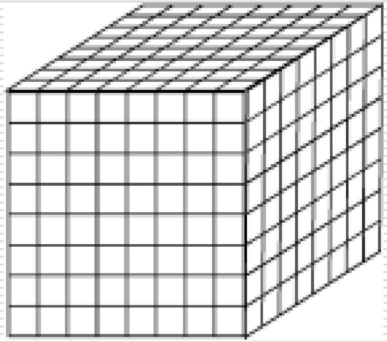


Resolve open issues of weak interactions

CKM matrix and CP violation (Matter-antimatter asymmetry in the universe)

Lattice QCD (I)

☐ Field theory on a 4-dim space-time Lattice suitable for numerical simulations



☐ Physical quantities given by *integral average* over quark and gluon fields defined on the lattice (Feyman path integral)

$$\left\langle O\left(U,\bar{\psi},\psi\right)\right\rangle = \frac{1}{Z}\int\prod_{\ell} dU_{\ell}\prod_{n} d\bar{\psi}_n d\psi_n O\left(U,\bar{\psi},\psi\right) e^{-S_{QCD}}$$

$$\left.\begin{array}{l}\text{Quark field } \psi_n \\ \text{Gluon field } U_\ell\end{array}\right\}$$

defined on the lattice

⇨ *large-scale Monte Carlo evaluation*

☐ Action is unique, i.e., *no issue of "modeling"*

(except for controllable discretization ambiguities)

$$S_{QCD} = \frac{1}{\alpha_s}\sum_{P} tr\left(U_{\ell_1}U_{\ell_2}U_{\ell_3}U_{\ell_4}\right) + \sum_{n,n'}\bar{\psi}_n D_{n,n'}\left(U\right)\psi_{n'}$$

Lattice QCD (II)

From computational point of view:

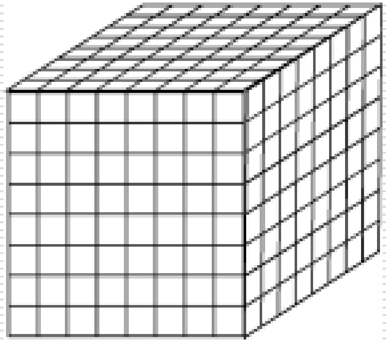
- Relatively simple calculational structure
  - Uniform mesh
  - Local interaction
  - Dominated by vector calculations

lattice spacing a

$$p_n \to \sum_{n'} D_{n,n'}(U)\, p_{n'}$$

⇒ *Ideal target of parallel computation with distributed memory*

- Requires much computing power due to
  - 4-dimensional Problem
  - Fermions (quarks) essential (determinant)
  - Physics is at lattice spacing a=0
  - Precision required
    (< a few % accuracy in many cases)



Computers for lattice QCD

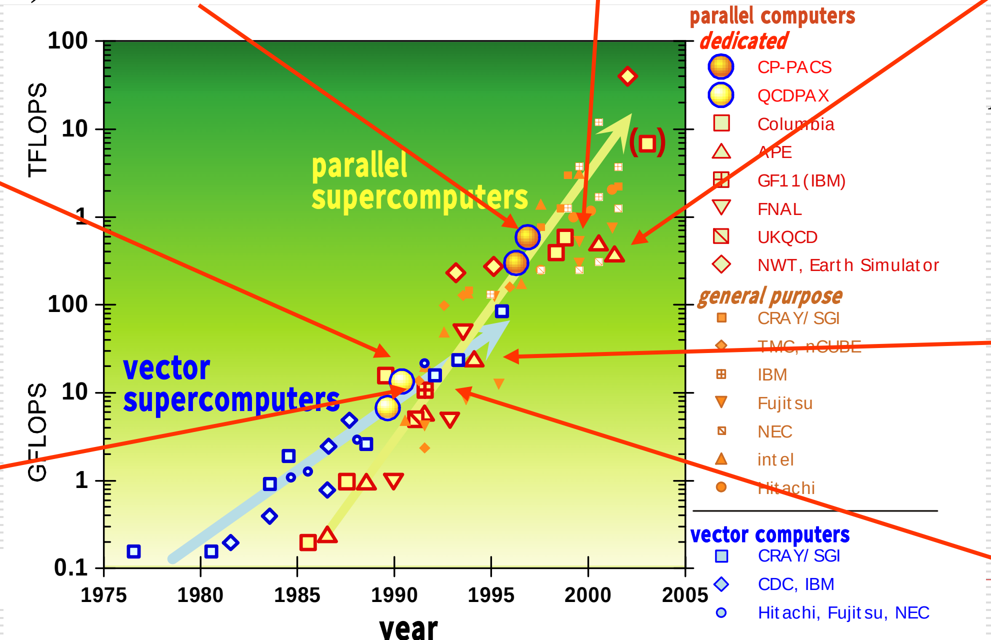
year	machine	peak
88-90	Columbia	16 GFLOPS
89-90	QCDPAX	14 GFLOPS
91	GF11	11 GFLOPS
88-94	APE / APE-100	25 GFLOPS
89-93	ACPMAPS	50 GFLOPS
96	CP-PACS	614GFLOPS
98-99	QCDSP	410, 600
00-01	APEmille	520 GFLOPS
03?	QCDOC	10Tflops
03?	ApeNext	5-10Tflops

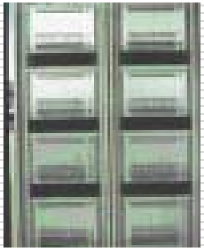

CP-PACS (1996) 614 GFLOPS


QCDSP (1998) 600 GFLOPS


APEmille (2000) 520 GFLOPS

lumbia (1990) 16 GFLOPS




APE-100 (1994) 25GFLOPS


CDPAX (1990) 14 GFLOPS

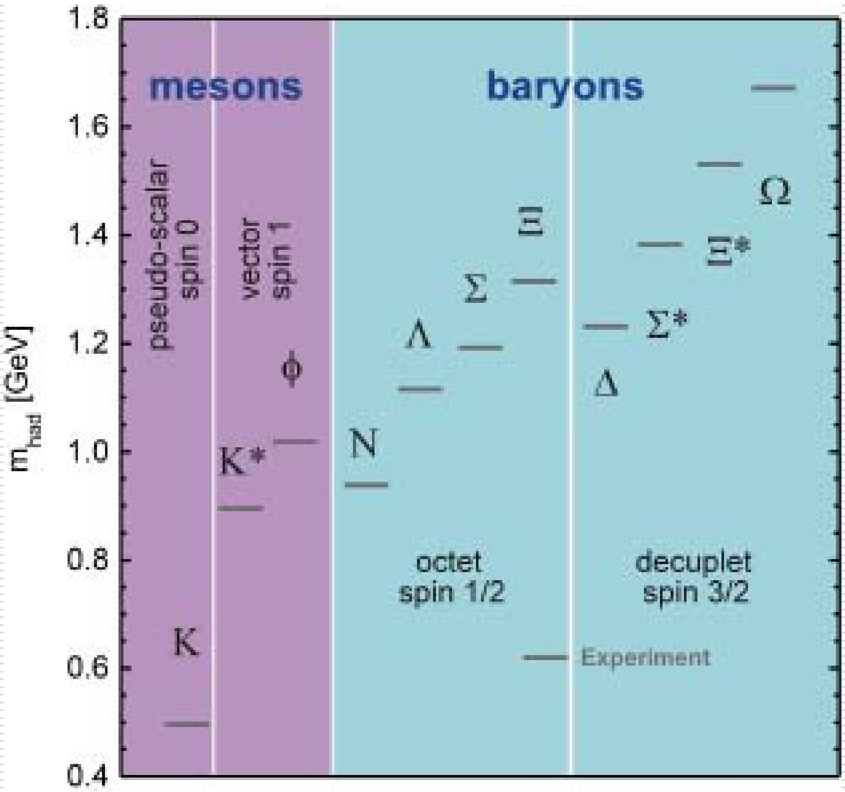
GF11 (1991) 11 GFLOPS

Selected Physics achievements

- Hadron mass spectrum
- Light quark masses
- Weak interactions of hadrons
    - $K \to \pi\pi$ decays and CP violation
    - Constraints on the CKM quark mixing matrix

Light hadron mass spectrum

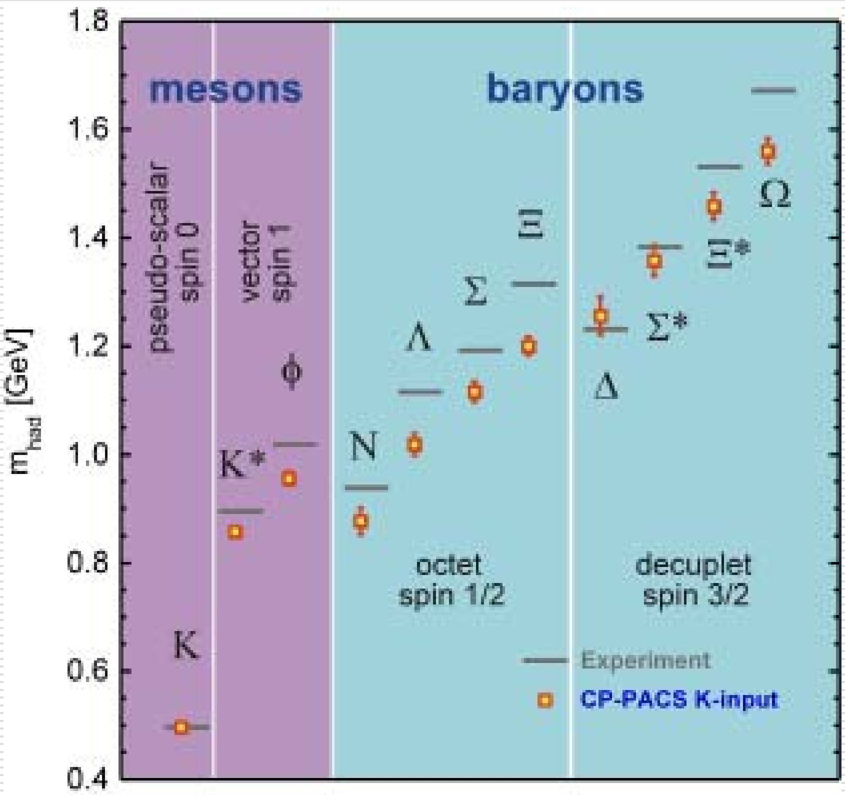
- ☐ Benchmark calculation to verify QCD
  - Pursued since 1981 (Weingarten/Hamber-Parisi)
- ☐ Essential to control various sysmatic errors down to a % level
  - Finite lattice size L>3fm
  - Finite quark mass mq→0
  - Finite lattice spacing a→0



Experimental spectrum

CP-PACS result for *the quenched spectrum*

- Quenched: quark-antiquark pair creation/annihilation (*sea quark effect*) ignored
- General pattern in good agreement with experiment
- Clear systematic deviation below 10% level
  - Indirect evidence of sea quark effect
- Completes the calculation pursued since 1981



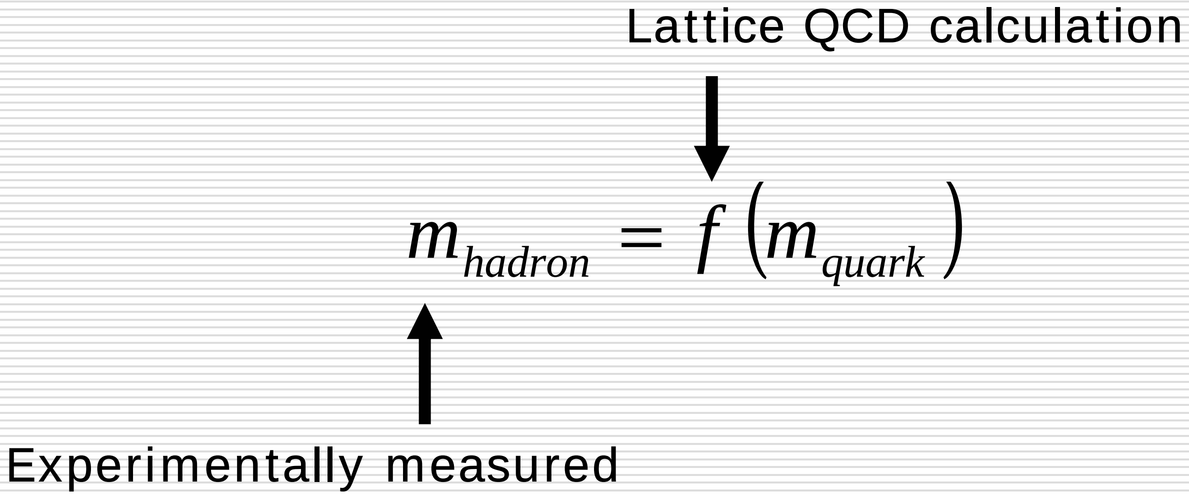
Calculated quenched spectrum

QCD simulation with dynamical quarks

- Spectrum of quarks
  - *3 light quarks (u,d,s)* *m < 1GeV*
    - *Need dynamical simulation*
  - 3 heavy quarks (c,b,t) m >1GeV
    - Quenching sufficient
- Dynamical quark simulation (full QCD)
  - costs 100-1000 times more computing power
  - Algorithm for *odd number of quarks* now developed
- *Two-flavor full QCD (since around 1996)* $N_f = 2$
    - u and d quark dynamical simulation
    - s quark quenched approximation
  - Number of studies: SESAM/UKQCD/MILC/CP-PACS/JLQCD
- *Three-flavor full QCD (since around 2000)* $N_f = 2+1$
    - s quark also treated dynamically
  - serious studies are beginning : MILC/CP-PACS-JLQCD

Determination of quark masses

- Fundamental constants of nature (like electron mass)
- Can not be measured by experiment since quarks are confined within hadrons
- *Theoretical determination from the relation of hadron mass as a function of quark mass is the only way*



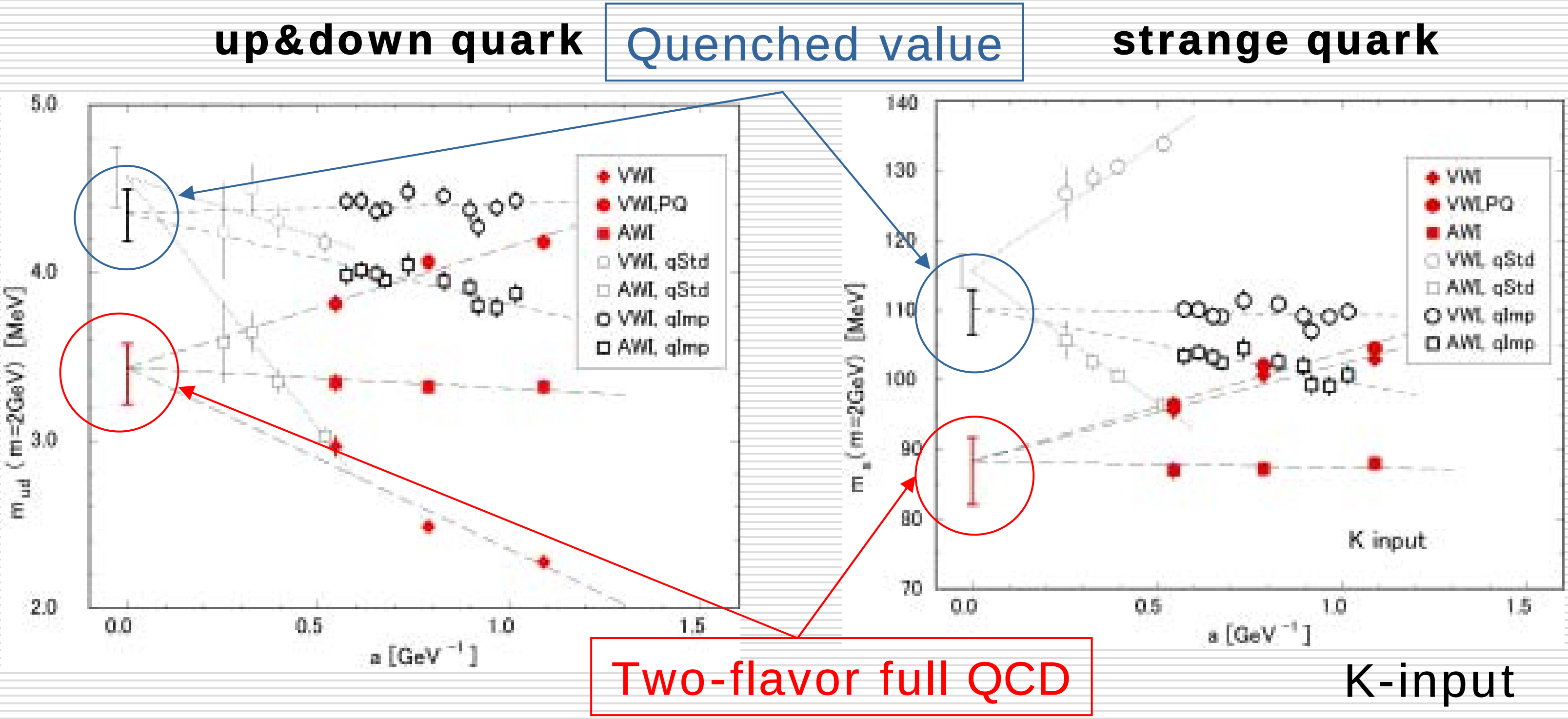
Lattice QCD calculation

$$m_{hadron} = f\left(m_{quark}\right)$$

Experimentally measured

Sea quark effects in quark masses

- Continuum extrapolation of light quark masses
  - Several methods yield a unique value in the continuum limit
  - Significant decrease by inclusion of sea quark effects



up&down quark

Quenched value

strange quark

Two-flavor full QCD

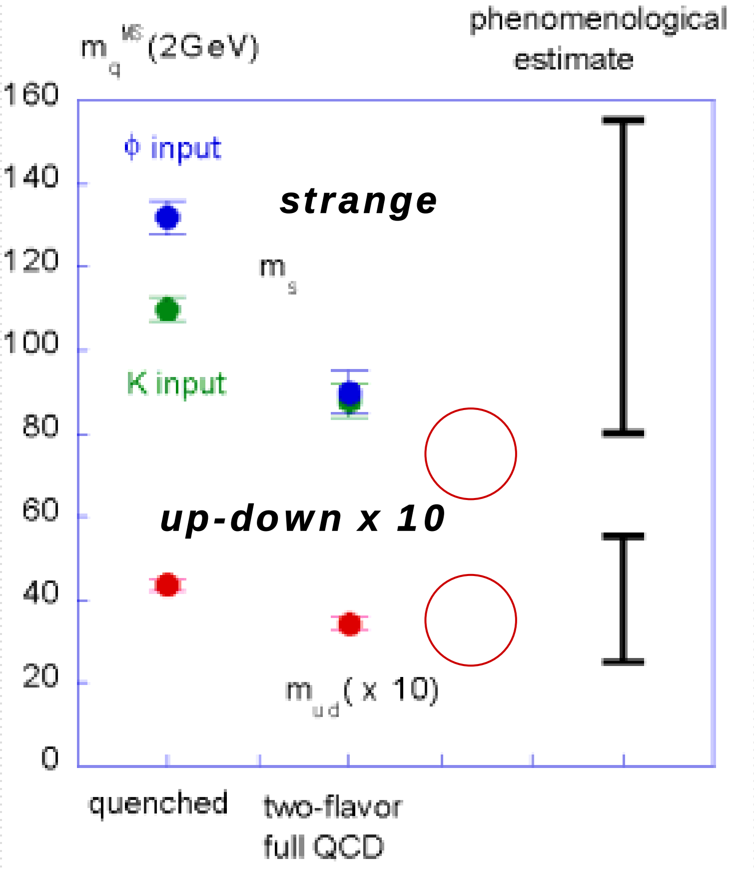
K-input

Light quark masses (u, d, s) $m_q^{\overline{MS}}(2GeV)$

- Significant sea quark effects
  - Large uncertainty (～20%) depending on input in quenched theory
  - Sizable decrease (～25%) from quenched to two-flavor full QCD
- Lighter than naïve quark model values
- Nf=3 simulations being pursued to obtain physical values of light quark masses,

e.g., Hein et al hep-lat/0209077

CP-PACS Collab. Hep-lat/0004010



Real world;three flavors?

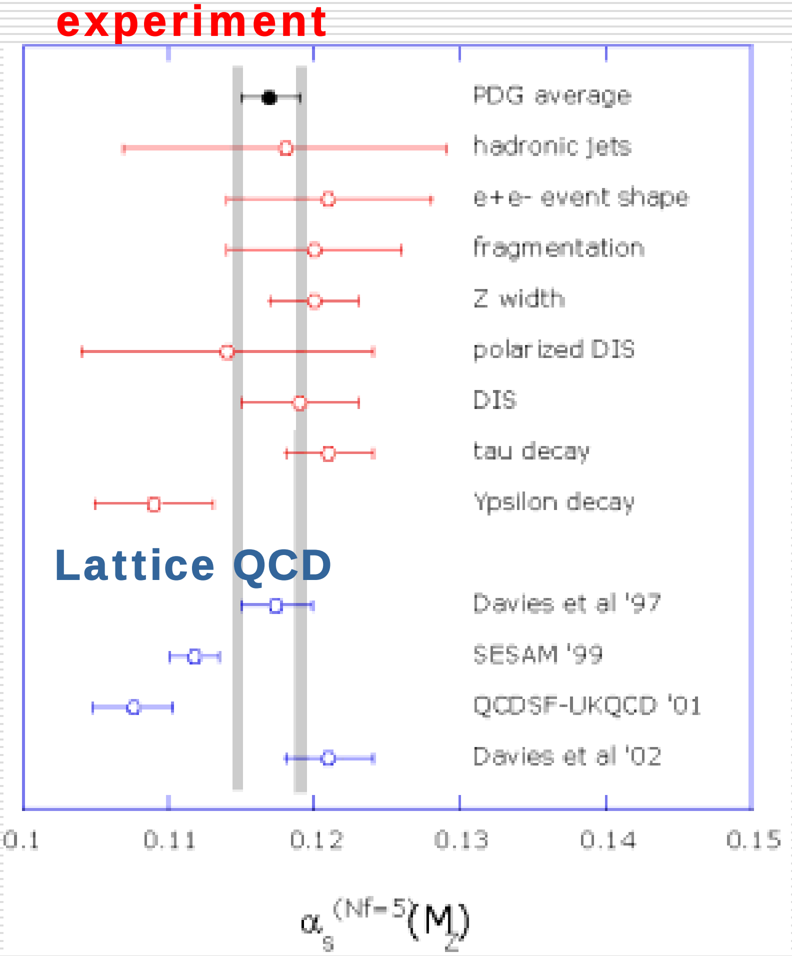
Strong coupling constant $\alpha_s(\mu)$

- Another fundamental parameter of QCD
  - determines the strength of strong interaction $\alpha_s(\mu) = \frac{g^2_{QCD}(\mu)}{4\pi}$
  - similar to determination of fine structure constant for electric charge

$$\alpha = \frac{e^2}{4\pi\hbar c} = 1/137.03599976(50)$$

- Large number of high energy determinations from experiments
- Lattice determination with three dynamical quarks still incomplete

Determination of $\alpha_s^{\overline{MS}}(M_Z)^{N_f=5}$



☐ Comments

- Davies et al ’97(hep-lat/9703010):

  Involved extrapolation of Nf=0(quenched) and Nf=2 data to Nf=3
- QCDSF-UKQCD ’01(hep-lat/0103023)

  Continuum estimate with systematic Nf=2 simulations
- Davies et al ’02(hep-lat/0209121):

  Preliminary result based on MILC **Nf=3** configurations at a=0.13fm

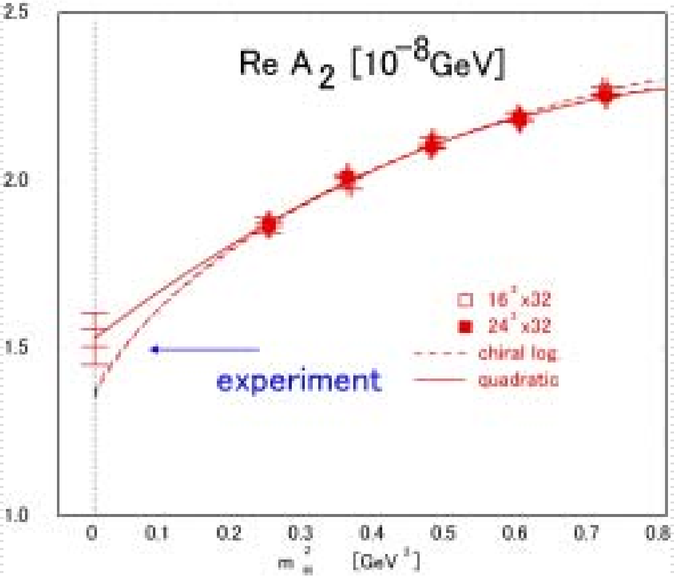
☐ *Systematic Nf=3 full QCD determination expected in a few years*

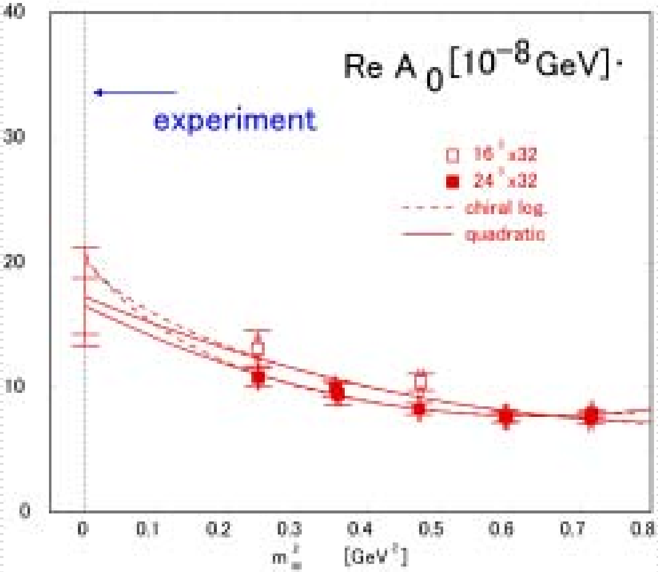
Δ I=1/2 rule and CP violation in K decays

- Weak interaction decays of K mesons
  - Δ I=1/2 rule $$\frac{\mathrm{Re}\,A_0\left(K \to \pi\pi(I=0)\right)}{\mathrm{Re}\,A_2\left(K \to \pi\pi(I=2)\right)} \approx 22$$
  - CP violation $$\frac{\varepsilon'}{\varepsilon} = \frac{\omega}{\sqrt{2}|\varepsilon|}\left[\frac{\mathrm{Im}\,A_2}{\mathrm{Re}\,A_2} - \frac{\mathrm{Im}\,A_0}{\mathrm{Re}\,A_0}\right]$$ $$= \begin{cases} (20.7 \pm 2.8)\times 10^{-3} & KTeV \text{ experiment } (FNAL) \\ (15.3 \pm 2.6)\times 10^{-3} & NA48 \text{ experiment } (CERN) \end{cases}$$
- Crucial numbers to verify the Standard Model understanding of *CP violation (matter-antimatter asymmetry)*
- Two large-scale calculations using domain-wall QCD
  - RIKEN-BNL-Columbia by QCDSP
  - CP-PACS

ΔI=1/2 rule

- Reasonable agreement with experiment for I=2
- About half of experiment for I=0
- RIKEN-BNL-Columbia obtains a somewhat different result (smaller I=2 and larger I=0)

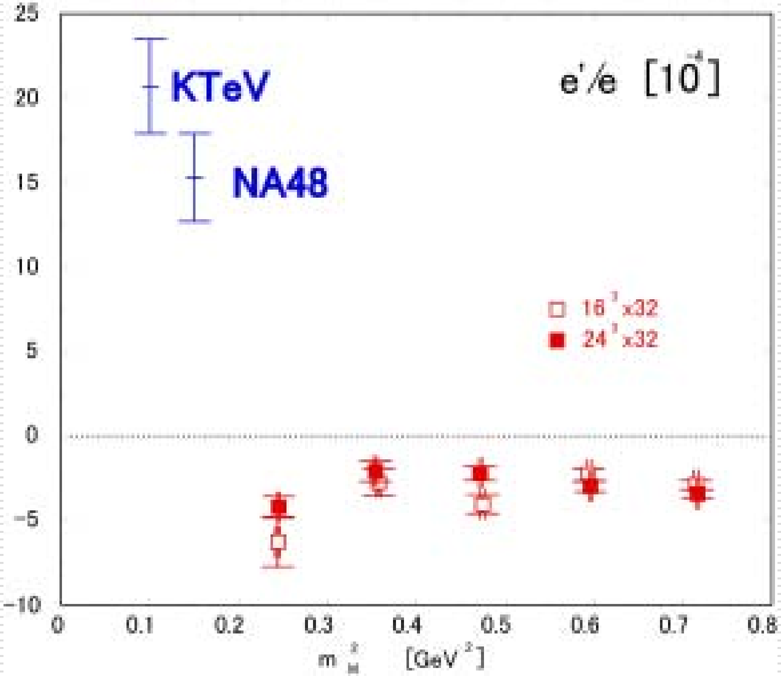




CP violation parameter ε'/ε

- Small and negative in disagreement with experiment
- Similar result from RIKEN-BNL-Columbia

$$\frac{\varepsilon'}{\varepsilon} = \frac{\omega}{\sqrt{2}|\varepsilon|}\left[\frac{\mathrm{Im}\,A_2}{\mathrm{Re}\,A_2} - \frac{\mathrm{Im}\,A_0}{\mathrm{Re}\,A_0}\right]$$



- Possible reasons
  - connected with insufficient enhancement of ΔI=1/2 rule
  - Method of calculation (K→π reduction) may have serious problems

- *Still a big problem requiring further work*

Constraints on the CKM matrix

$$\begin{pmatrix} u \\ c \\ t \end{pmatrix} \Leftrightarrow \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \begin{pmatrix} d \\ s \\ b \end{pmatrix}$$

$$= \begin{pmatrix} 1-\lambda^2/2 & \lambda & A\lambda^3(\rho - i\eta) \\ -\lambda & 1-\lambda^2/2 & A\lambda^2 \\ A\lambda^3(1-\rho - i\eta) & -A\lambda^2 & 1 \end{pmatrix} \begin{pmatrix} d \\ s \\ b \end{pmatrix} + O(\lambda^4)$$

- Controls mixings among quarks
- *Controls CP violation (matter-antimatter asymmetry)* η

Constraints on the CKM parameter (ρ, η)

B factory experiment
(KEK-SLAC) '01-'02

status 2002

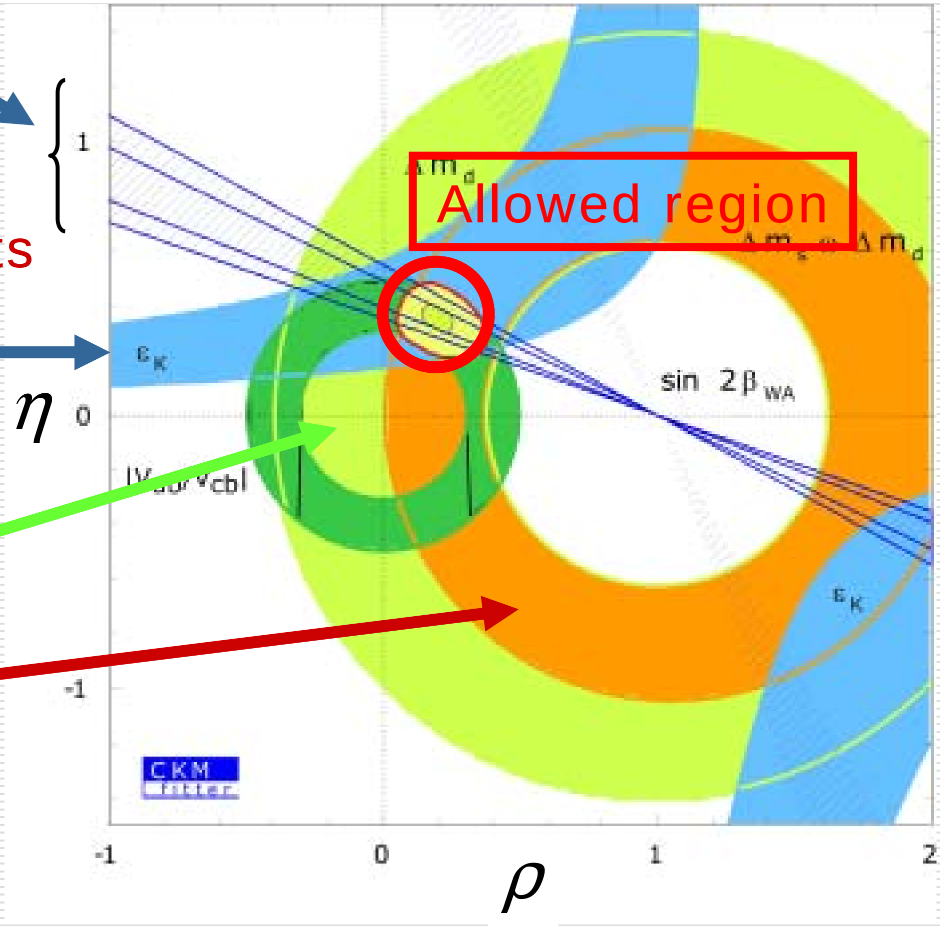
http://www.ckmfitter.in2p3.fr/

Lattice QCD +
well-established experiments

$$\hat{B}_K = 0.87^{+0.06}_{-0.13}$$

$$f_{B_d}\sqrt{B_{B_d}} = 0.227(37)^{+0}_{-34}\,GeV$$

$$\xi = 1.16(5)^{+24}_{-0}$$



Future direction of lattice QCD

- From 2-flavor QCD to 3-flavor QCD
  - Dynamical treatment of all light quarks (u, d, s)
  - Realistically light quark simulations

Polynomial HMC algorithm

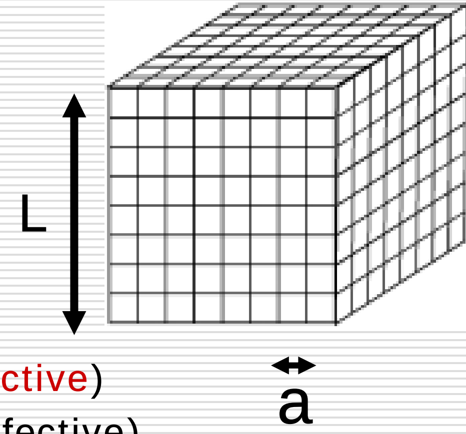
$$\frac{m_\pi}{m_\rho} \approx 0.6 \ (m_\pi \approx 500\ MeV)$$

$$\Rightarrow \frac{m_\pi}{m_\rho} \approx 0.2 \ (\text{experiment})$$

- From non-chiral to chiral action for quark
  - Domain-wall/overlap/perfect actions
  - Theoretically the formalism of choice but requires O(10) times more computing

⇨ *realistic and*
exact simulation of QCD

Scale of QCD simulations



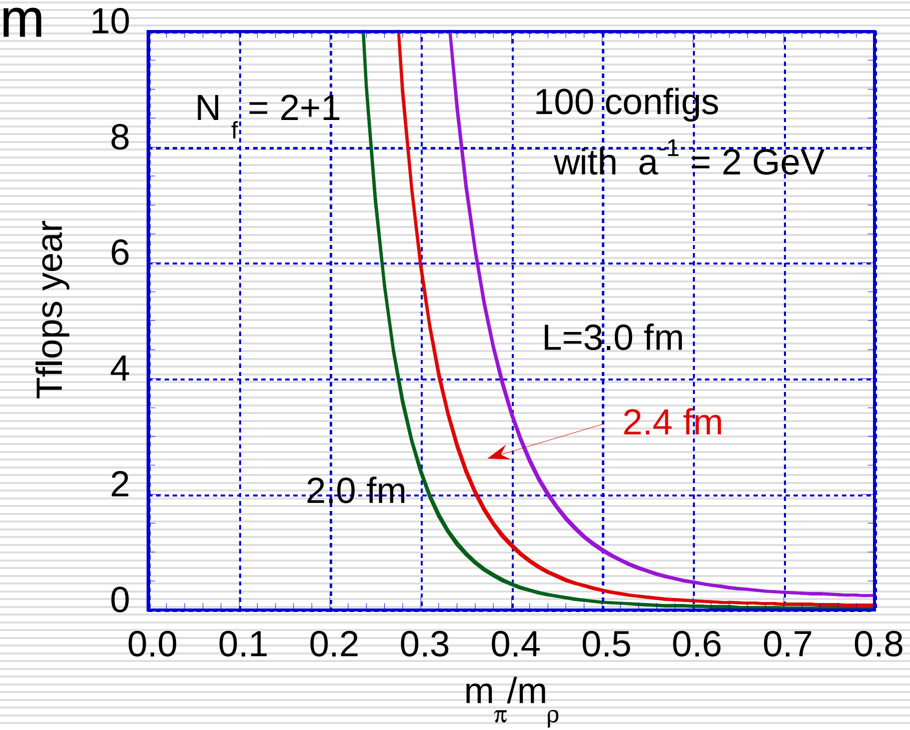
- Typical lattice size
  - Quenched QCD 64^3x112
  - 2-flavor Full QCD 24^3x48
- Total CPU time with CP-PACS
    - 0.6Tflops peak
    - 53% of peak for quenched QCD (0.32Tflops effective)
    - 34% of peak for 2-flavor full QCD (0.20Tflops effective)
  - Quenched QCD 199 days of full machine
  - 2-flavor full QCD 415 days of full machine
  - K decay 180 days of full machine
- *Scaling law for 2-flavor QCD*

$$\#FLOP's = C \cdot \left[\frac{\#conf}{1000}\right] \cdot \left[\frac{m_\pi / m_\rho}{0.6}\right]^{-6} \cdot \left[\frac{L}{3\,fm}\right]^{5} \cdot \left[\frac{1/a}{2GeV}\right]^{7} Tflops \cdot year$$

$$C \approx 2.8$$

First step of serious 3-flavor simulations

- ☐ Polynomial HMC algorithm
- ☐ Assumption for Scaling law for 3-flavor QCD
  - FLOPS=1.5*(2flavor case)
- ☐ O(5-10)Tflops computer needed for L=2.4fm simulations with 100 samples



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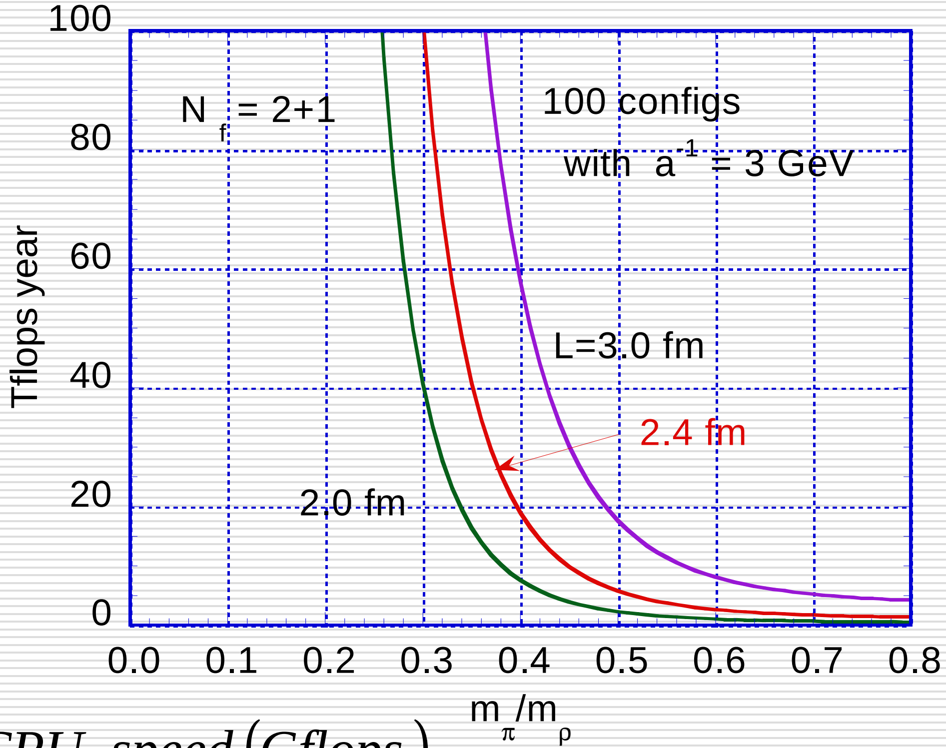
- Earth simulator well suited for the job
- also QCDOC (10Tflops)/ApeNEXT (5-10Tflops) expected in fall 2003

Future requirements toward solving QCD

- Total speed of O(100)Tflops and more

- Fast network scaling with CPU speed

with 50% finer lattice mesh



$$\frac{communication\ time}{calculation\ time} \approx \frac{1}{2\times(lattice\ \ size/node)} \times \frac{CPU\ \ speed\,(Gflops)}{network\ \ speed\,(GB/\sec)}$$

Worldwide prospects

- Regional developments and competition
  - USA/Europe/Japan

    →Asia-Pacific:Korea/Taiwan/China/Australia/Japan/
- International collaboration
  - Sharing of resources and collaboration
    - 1st International Workshop on Lattice Data Grid (19-20 Dec 02)

Conclusions

- Significant progress over the last two decades
  - Large body of physics results relevant for experiment
  - Development of parallel computers hand in hand
- Entering the phase where truly realistic simulations are becoming possible due to
  - Algorithm developments
  - O(10) Tflops computers
- With futher enhancement of computer power, definitive prospect toward exact QCD predictions with realistic quark spectrum in the coming decade